

ON A PARADIGM FOR MATHEMATICAL MODELING

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Abstract

The role of mathematical modeling in science is explored with emphasis on its creative aspect — the modeler's art. A paradigm is described which emphasizes the cyclic nature of the process and whose components are abstraction, prediction, interpretation, testing and revision. Abstraction and interpretation allow movement between the real-world and the symbolic, prediction occurs in the mathematical realm and is governed by its laws, testing occurs in the real-world and provides the basis for revision.

The abstraction step requires inductive insight and some recent techniques for its teaching are described. The prediction step is deductive and the choices between stochastic and deterministic, between analytic and simulative, and between discrete and continuous formulations are discussed. Finally, an analysis of the weight of model predictions is given.

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1. Introduction

Models are, for the most part, caricatures of reality, but if they are good, then, like good caricatures, they portray, though perhaps in distorted manner, some of the features of the real world.

Thus Mark Kac [1969] elegantly summarizes the role of mathematical models in science. It is my purpose here, to explore that role, but since such exploration must follow a personal course, shaped by the author's experience, I shall no doubt leave important issues untouched. For example, I shall avoid a discussion of the role of formal axiom systems in mathematical modeling. Such a discussion would be too technical for our purposes and is well treated elsewhere, e.g., Maki and Thompson [1973] or more thoroughly in Wilder [1965]. On the other hand I shall emphasize the creative aspect of the modeler's art. Much of what I say here will have been said before, but it is nevertheless appropriate to recall it on this opening day to establish a frame of mind for the remainder of the workshop. My experience in presenting some of these ideas to an introductory modeling course, however, prompts the caveat that it might be even more appropriate to have saved this discussion for the closing day!

1.1. Some Definitions

To give any definition of a model is to invite exception, but a reasonable attempt is represented by Friedenbergs [1968] universal definition of a model as a "simplified representation of a real physical system". We shall here limit our discussion of models to mathematical models, for after all, the double helix of molecular genetics is too a model as are wind tunnel prototypes.

Bender [1975] somewhat circularly defines a mathematical model as "an abstract, simplified, mathematical construct related to a part of reality and created for a particular purpose", while Kac [1969] simply takes mathematical models to be "models which can be described symbolically and discussed deductively".

1.2. The Value of Modeling

Why build mathematical models rather than study Nature first-hand? Again we turn to Kac [1969] who observes that the primary purpose of modeling is to "polarize thinking and to pose sharp questions". As a statistician, I would complete the statement by observing that the sharp questions are then put to Nature directly using carefully designed experiments.

In mathematical modeling we must be precise. That we are compelled to simplify our view of a physical system, to strip away all but the most essential features of reality in order to be able to formulate a model precisely, can expose the fertile ground required for the emergence of deeper insights.

In formulating a model mathematically, we provide a language with which we can manipulate (subject to the laws of mathematics and logic) relationships amongst the primitives of our subject matter, to establish, unambiguously, implications of the theory on which the model is based, and so to test that theory. The method forces us to identify and label assumption, supposition and idealization. Modeling can also be used to synthesize and organize existing knowledge, to integrate independent findings and thus assess their compatibility.

Finally, modeling provides an economy of thought and a common language for scientists in diverse disciplines. Lurking behind every biological model is an economic model - a change of nouns effects the conversion.

1.3. Two Motivations

There are many ways in which one can classify mathematical models: simple versus complex, descriptive versus conceptual, analytic versus simulative, cause-effect versus effect-effect, deterministic versus stochastic, and so on. Perhaps the most important such classification is according to purpose. While we agree with Kac [1969] as to the general intent of modeling, it is nevertheless convenient to classify models as either motivated by a desire to understand the real world or motivated by a desire to provide a basis for prediction and (perhaps) control. An example of the latter motivation is a wish to predict the effect on the dynamics of some biological population of a proposed environmental perturbation. This can sometimes be done (and is often attempted, e.g., with linear regression models) with little biological understanding.

A similar scheme, described by Lucas [1964] classifies models as rational or empirical. Rational (or heuristic) models are Gedanken models, derived from theory and conjecture about the real system, making careful use of known characteristics of the system, and couched in meaningful terms. Empirical models to the contrary are exemplified by "curve-fitting" and pay little attention to underlying mechanisms. Of course, most models while ideally rational, have empirical components, reflecting lack of theory and the modeling process encourages us to identify these gaps. Lucas [1964] cautions us to introduce "as much rationality as possible into all models used", insofar as such models are likely to also prove better predictors than their empirical counterparts when extrapolating outside the data regions on which the empirical models are based.

2. Strategies for Modeling

The quality of a modeling effort can be measured in several ways, but the final test is how able a model is to make correct predictions. Nevertheless,

numerous attributes of models can be identified and an appropriate modeling strategy should be determined by the specific objectives of the investigation.

Several authors have proposed criteria for good models and we list a few of them. Levins [1966] argues, in the context of population biology, that models should be constructed to maximize generality, realism and precision. Noting that these are competing objectives, he gives examples in each of which the modeling strategy is to sacrifice one quality to the other two.

Generality, also referred to as robustness, allows a model to make predictions over broad regions of time or parameter values. Robust models are relatively insensitive to minor changes in assumptions. Indeed, the reality which a model attempts to mimic may itself be quite sensitive to certain types of perturbation, and we should not fault a model of such a system for sharing this property. Thus a dynamical model of a commercial fishery might become valueless for prediction in the face of a discontinuous change in the environment brought about by a changed political condition, for example international fishing regulations.

The most visible property of a model is the extent to which it is realistic - to which it does not make simplifying assumptions. Equivalently, this is a measure of the model's complexity, and it is the level of resolution required by the subject matter that must determine an appropriate trade-off between tractability and reality. As we will observe later, modeling is a cyclic process, commonly beginning with simple models and adding complexity (by dropping assumptions) as understanding is gained and new questions raised. It is crucial that the modeler be able to move easily between the model and the real world, in order to assess sensitivity and to revise.

In many modeling circumstances, it is precision which can be sacrificed since often only qualitative predictions are required - Will the proposed perturbation

make the population rise or fall? — Then too, the quality of data on which parameter estimates are based may not justify an attempt at precise prediction.

Other characteristics of good models have been given by Morris [1967] who lists:

Relatedness. How many previously known theorems or results does the model bring to bear upon the problem?

Transparency. How obvious is the interpretation of the model? How immediate is its intuitive confirmation?

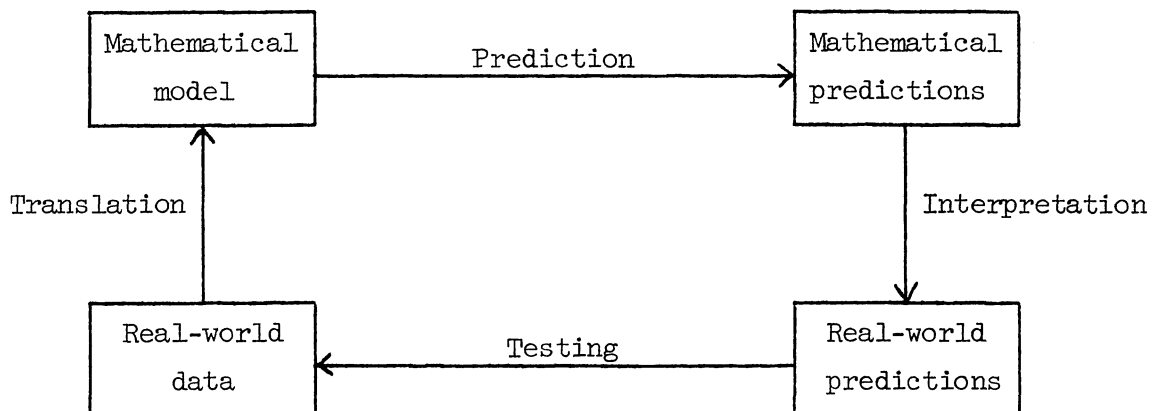
Fertility. How rich is the variety of deductive consequences which the model produces?

Ease of Enrichment. What difficulties are presented by attempts to enrich and elaborate the model in various directions?

Finally, modeling strategy also includes choice of mathematical tools — stochastic or deterministic, differential equations versus difference equations, etc. But we postpone this discussion for later attention.

3. A Paradigm

Although there are numerous variants in the literature, the components of the mathematical modeling process are perhaps most clearly depicted by Roberts [1976] as follows:



The figure emphasizes the cyclic nature of the process, and our choice of a starting point for its discussion is arbitrary.

We shall, in fact, begin with the real-world system to be modeled. By a procedure which Roberts calls translation and which others call abstraction, the modeler represents the real-world symbolically. Some writers here insert a subject matter theory — a "real-world model" — between the real-world and the mathematical model. This is the inductive step and the one which cannot be taught except perhaps by apprenticeship. It is an art and at best we might provide conditions under which it will flourish.

The predictive step on the other hand is deductive, and it is here that we can bring all the power of existing mathematics to bear to arrive at the logical implications of the mathematical model. These implications are then translated back to the language of reality by interpretation of the symbols. This provides the real-world predictions and is the entry point for the statistician who designs real-world experiments with which to test the predictions. The adequacy of the model is thus assessed, our understanding of reality is modified, and the cycle begins anew.

We shall, in what follows, look a bit more closely at each step in the process.

4. Abstraction

The translation or abstraction step which takes us from the real-world to the mathematical model has two components — the inductive insight and the choice of mathematical formalism. The inductive aspect is the creative one, the one exceptionally difficult to teach, the one even difficult to describe. The choice of mathematics, on the other hand, I will soon argue, is largely preconditioned.

4.1. Induction

Leon Eisenberg [Maugh, 1974] has observed that the teaching of creativity is complicated by the fact that insight is preverbal and thus any verbal description of the conditions leading to the birth of an original idea may well be faulty. Paul Halmos [1968] in a beautiful lecture titled "Mathematics as a Creative Art", described as follows the labor pains of insight as experienced by a mathematician:

The mathematician at work makes vague guesses, visualizes broad generalizations, and jumps to unwarranted conclusions. He arranges and rearranges his ideas, and he becomes convinced of their truth long before he can write down a logical proof. The conviction is not likely to come early — it usually comes after many attempts, many failures, many discouragements, many false starts. It often happens that months of work result in the proof that the method of attack they were based on cannot possibly work, and the process of guessing, visualizing, and conclusion-jumping begins again. A reformulation is needed — and — and this too may surprise you — more experimental work is needed. To be sure, by "experimental work" I do not mean test tubes and cyclotrons. I mean thought-experiments. When a mathematician wants to prove a theorem about an infinite-dimensional Hilbert space, he examines its finite-dimensional analogue, he looks in detail at the 2- and 3-dimensional cases, he often tries out a particular numerical case, and he hopes that he will gain thereby an insight that pure definition-juggling has not yielded. The deductive stage, writing the result down, and writing down its rigorous proof are relatively trivial once the real insight arrives; it is more like the draftsman's work, not the architect's.

Induction and creativity have, of course, long been subjects for philosophers and psychologists, and we do not pretend to those titles here. However, we have seen recent attempts to teach the mathematical modeler's art in college curricula, and I should like to describe some of the techniques proposed.

Frauenthal and Saaty [1976] offer a collection of apparently difficult and confusing problems. The problems share the property that a crucial insight suggests a mathematization which renders the problem trivial, usually soluble without pencil and paper. A sample illustrating the role of symmetry and exemplifying analytic versus synthetic thinking follows:

The Cup of Coffee and the Cup of Milk. Imagine you are given a cup of coffee and a cup of milk, with equal amounts of liquid in the two cups. A spoonful of milk is transferred from the milk cup to the coffee cup, stirred and then a spoonful of the mixture is returned to the milk cup so at the end the amount of liquid in the two cups is still the same. Is there more milk in the coffee cup or more coffee in the milk cup or what?

Most people say there is more milk in the coffee cup, a few say the reverse and still fewer say they are equal. The feeling about this problem is that the first transfer of milk to the coffee cup so dilutes the spoonful in coffee that the next transfer of the mixture cannot take back much of it, hence leaving more milk in the coffee cup than coffee in the milk cup. Of course, not being able to take back much of it should make it possible to take a lot more coffee in the spoonful. But people don't think of it that way.

Insight: Notice that whatever amount of milk is missing from the milk cup is replaced by an equal amount of coffee (and vice-versa) because at the end each cup has the same amount of liquid with which it started.

Solution: It is therefore obvious that there are equal amounts of coffee in the milk and milk in the coffee.

One can verify this with algebra but with more effort. However the algebra assumes homogeneity of the mixture in the coffee cup after stirring. This assumption is artificial but unfortunately is needed to carry out the algebraic argument that the second spoonful has the same ratio of coffee to milk as there is in the entire coffee cup.

The object of the approach is to " ... illustrate to the student an incisive way of thinking which can be carried over into more difficult problems ... to improve intuition by alerting the student to principles which operate in a domain which is apparently finer than that encountered in daily discourse and in common thought."

Morris [1967] suggests a procedure for modeling which includes the following recommendations:

- a. Factor the problem into simpler ones.
- b. Establish a clear (but perhaps tentative) statement of the deductive objectives. The final objective may prove to have been unforeseen.
- c. Seek analogies. This too is an intuitive step, but worth focusing on.

- d. Consider a specific numerical instance. This may uncover hidden assumptions, suggest generalization and at least provide initial notation.
- e. Establish symbols. This requires that we clearly identify the objects to be mathematized. This often involves idealizations that the experienced modeler performs by second nature but should be called to the attention of the novice. For example in studying spatial pattern, to identify plants as points is an idealization.
- f. Write down the obvious. That is, write in terms of the symbols the obvious aspects of the numerical example in hopes of suggesting generalization.
- g. If a tractable model is obtained, enrich it. Otherwise, simplify. We shall return to this point in our discussion of model revision.

Pollock [1976] has adapted Morris' principles to create, in coursework fashion, a modeling studio. He argues that if modeling is an art, then the principles for teaching the traditional arts of music, painting and sculpture should apply. Although I will not detail those principles here, an example is the encouragement of excess. This might be achieved by extremes of color or size in the visual arts - to test the limits of the artist and the medium. The implication for mathematical modeling is that such daring invites fresh perspectives and innovative approaches. Another important ingredient of Pollock's modeling studio is criticism by other modelers and by oneself.

4.2. Choice of Tools for Deduction

The second part of the abstraction step of the modeling paradigm is the choice of a mathematical formulation - the choice of tools for the deductive step. An appropriate choice is of course not unique, and in fact is largely conditioned by

the modeler's mathematical training. I saw an excellent illustration of this when Pollock, in lecturing to a diverse collection of faculty and students from applied mathematics, statistics and operations research, proposed a phenomenon to be modeled and invited the audience's insights. The mathematicians saw the situation as a natural for description by a system of differential equations, while the statisticians envisioned a birth and death stochastic process and to the operations researchers, it was obvious that the appropriate tools were those of queuing theory.

4.3. Stochastic versus Deterministic Models

As promised at the outset, this discussion is following a personal course, and so I should like now to briefly consider the subject of stochastic versus deterministic model formulations. Variability in the biological world is well-known to all of us. Maynard Smith [1974] in the context of mathematical ecology claims that deterministic models fail to mirror reality in assuming infinite population sizes and in ignoring random fluctuations in the environment. May [1974] expands, observing that "birth rates, carrying capacities, competition coefficients, and other parameters which characterize natural biological systems all, to a greater or lesser degree, exhibit random fluctuations." Ehrlich and Birch [1967] boldly assert "models must be stochastic not deterministic."

If stochastic models are admittedly more realistic, what then the justification for deterministic approaches? A primary one is tractability. By itself, of course, mathematical convenience has no place in model building, but deterministic models have often proven adequate for mimicing biological systems and providing biological insights. Deterministic models are often taken as first approximations to stochastic models, and study of deterministic models can also provide answers to questions about the behavior of stochastic ones. For example, May [1971a,b] describes an m-species population model with random environment showing that the

conditions for the existence of an equilibrium probability distribution are identical to those for a stable equilibrium in the deterministic case. He furthermore concludes that if complex natural ecosystems are stable then the interactions in them are essentially non-random.

In a recent series of publications (e.g. Oster [1974]) simple deterministic models have been presented which exhibit behavior described as chaotic. That is, behavior in which the time path of the system could be taken for a sample path of a stochastic process. The implications of the ability to mimic stochastic fluctuations with deterministic models are not yet well studied.

Voltaire has said "Chance is a word void of sense; nothing can exist without a cause." Charles Dickens would disagree: "Accidents will occur in the best regulated families." It is beyond our scope to address seriously the fundamental but irresolvable issue of determinism versus indeterminism inasmuch as it is an issue which we hold is largely irrelevant to applications. That is, even in a deterministic universe, in which (I quote Bartlett [1960] after Schrödinger [1944]) " ... a multiplicity of detailed causes is operating to produce the observed broad class of events, it is often an economy of thought in the sense of Mach to ignore these and appeal merely to the operations of chance and the laws of averages." Thus, for example, in coin tossing or gamete pairing, even if we could argue that sufficient knowledge of the physical forces surrounding the event would completely determine the outcome, nevertheless from our level of resolution, we perceive the process as random.

In his treatment of the role of stochastic elements in biological models, Lucas [1964] expands on and formalizes these notions by proposing that the universe, which clearly possesses deterministic features, might also possess truly random ones, and if so, these would be characterized by inherent unexplainability and

thus be outside the realm of science. However, because of our current state of ignorance, or because of our failure to take certain knowledge into account, some of the deterministic features appear to us as random. To these, Lucas ascribes the name pseudo-random and defines the role of science as that of diminishing the amount of pseudo-randomness in the world, while true randomness, if it indeed exists, sets the bounds on explainability and predictability.

4.4. Simulation Models

When the mathematical problems associated with a model are too difficult to handle or there is a lack of fundamental theory, the modeler may turn to simulation. The role of the "pilot plant" for simulation in physical model building is played by the computer in mathematical model building. We shall not pursue the subject at length here, but would observe that simulation models tend to share the weaknesses of all empirical models. In ecosystem simulation models for example, there are often huge numbers of parameters, and many different sets of their values, though theoretically contradictory, may adequately simulate observed systems.

Advantages of simulation modeling are that they allow us to deal with much more complex systems than we could by analytic means, and that they can usually be designed to allow easy variation of parameter values, thus enabling assessment of sensitivity of the modeled system to its parameters.

4.5. Discrete or Continuous?

As a final note on the choice of mathematical tools I would call attention to the choice between discrete and continuous formulations for a model. The distinction arises in many settings. In studying spatial pattern in plant communities for example, we decide between number of stems and percent cover. In stochastic process models we choose between discrete and continuous states as well as between

discrete and continuous time. In deterministic models, the choice of discrete or continuous time becomes one of difference equations or differential equations.

Difference equations are usually viewed as convenient tools for approximating solutions to differential equations, which are of the primary interest. However, for many biological situations, it is the discrete formulation which is in fact the more realistic, the differential equations model being the approximation. A difficulty which arises when using differential equations representations of discrete phenomena is that a given differential equation corresponds to many difference equations, all with the same limiting differential equation, but themselves perhaps having widely different solutions. Some examples of the implications of this fact are given in the expository works of Van der Vaart [1973] and of Frauenthal [1976].

5. Mathematical and Real-World Predictions

We now apply our mathematical tools to the mathematical model to make mathematical predictions. The innovative part here is deciding on the subject matter questions to ask in the mathematical language. These predictions are then translated into the subject discipline to produce real-world predictions. Note that we do not here claim to real-world explanation — only prediction. As we shall emphasize later, different models may make identical predictions but provide different explanations. As Bender [1975] says, "The mechanism is irrelevant when dealing with predictions, but the nature of the mechanism is the heart of an explanation."

6. Model Testing

The final step in the modeling cycle is to compare model prediction with reality. This typically requires experimental design and statistical inference, which topics we shall not pursue here. We only note in this regard that a decision

must be reached as to how consistent with reality the model need be. This, of course, is determined by the reason for which the modeling effort was mounted. It should be emphasized that statistics is no substitute for the experienced scientist's intuition and wisdom of subject.

The question of whether a model is "right" lies outside of mathematics, and in some sense no model can be right. A prediction is correct only insofar as its mathematical counterpart is logically deduced from the axioms of the model. A conclusion derived from a model with gross assumptions is weak. A conclusion derived from a general model and insensitive to its assumptions or one corroborated by several models is robust.

There are numerous illustrations of the fact that several sets of underlying assumptions about a real phenomenon can lead to the same mathematical model, and thus the same predictions. It follows that even if a model is consistent with observation, it cannot be concluded that the assumed mechanisms on which the model is based are realistic.

One of my favorite such illustrations provides several sets of assumptions -- mutually contradictory -- for the spatial distribution of cabbage butterfly eggs on individual cabbage plants. One model proposes that adult female butterflies visit individual plants "at random", laying clusters of eggs. The environment is homogeneous in that all plants are equally attractive to the females. It is also supposed that the number of eggs in a cluster follows the same probability distribution for each cluster, and that the number of eggs in a given cluster is neither dependent on the number in any other nor on the number of clusters.

Contrary to the assumptions in the first model, a second supposes that eggs are not laid in clusters, but are spatially distributed at random on the cabbage plants. Furthermore, unlike in the first model, individual heads are not equally

attractive to the female butterflies, differing in size, condition and location (e.g., border versus interior of the plot or orientation with respect to the sun) and so the mean number of eggs varies from head to head.

Connecting the biological assumptions to mathematical ones leads us to conclude for both models that the number of eggs per plant should follow a negative binomial distribution, a prediction well confirmed by experiment (Harcourt [1961] and Kobayashi [1965]). Thus additional information would be required to decide between the two proposed mechanisms (neither of which need, of course, be correct). We emphasize that the biological assumptions on which the two models are based are not only different but are in fact contradictory. In the absence of additional information we might, nevertheless, make predictions about, say, the mean number of eggs per plant and thus about future butterfly population sizes. Such predictions could have implications for control decisions with important economic consequences even with the mechanism not fully understood.

For the curious, we remark that for this particular population, experiments have been performed in a net house to observe the detailed behavior of the female cabbage butterfly (Kobayashi [1966]). Peripheral plants and those nearer the light source were favored, but under uniform light conditions, the butterflies visited interior plants at random (Poisson). The independence assumption made in the first model was also tested and found tenable. Thus the first model proved the more appropriate description of the biological mechanism. A third set of assumptions about the cabbage butterfly system also leading to the negative binomial distribution, together with the mathematical details for all three models, may be found in Solomon [1976]. An additional collection of three temporal (as opposed to spatial) negative binomial models also appears there.

7. Model Revision

We have now come full circle and the path of science directs us to revise hypothesis, modify the model and begin anew. We recall that the last step in Morris' [1967] modeling scheme enjoins us to enrich a tractable model, simplify an intractable one. He lists as means of simplification: "making variables into constants; eliminating variables; using linear relations; adding stronger assumptions and restrictions; suppressing randomness". To enrich we perform the opposite modifications.

We close with the injunction that we must all be alert for new tools for the modeling studio and wary of stagnation in our modeling. New mathematics (the finite element method) or new ways to use existing mathematics (catastrophe theory) should continuously enrich our repertoire. (See Williams [1977] for a somewhat unorthodox expansion of these comments.)

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